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We study “internal” work optimization over the energy levels of a generic hot quantum Otto engine. We find universal features in the efficiency that resembles the classical “external” power optimization over the coupling times to the thermal baths. It is shown that in the ultra hot regime the efficiency is determined solely by the optimization constraint, and independent of the engine details. We show that for some constraints the radius of convergence of the perturbative approach used in the classical analysis is zero even for very arbitrarily low efficiencies at small temperature difference.

Carnot’s discovery of a universal efficiency upper bound for heat engines had a profound impact on physics and engineering. Yet, in practice to approach this efficiency bound the system needs to be reversible and that leads to infinitely slow cycle time and vanishing power output. This motivated extensive studies under the title of “finite-time thermodynamics” (see [1, 2] for review articles). More importantly, efficiency is only a secondary design goal. First the engine must be capable of doing the task it is designed to: lifting a weight in a given time, accelerating a car etc. In general the efficiency depends on the heat transfer mechanism between the system and the bath. Nonetheless, some universal features were discovered when the power output is maximal. In this work we study the universality of efficiency at maximal output of quantum Otto engines. In the engines studied here, the working substance is a single particle that constitutes an N -level system. In the adiabatic stroke of the quantum Otto engine the levels of the particle must be varied in time. In real systems this level variability is limited by practical considerations. For example in Zeeman splitting the maximal gap is determined by the maximal available external magnetic field. In other systems it may be the power of the laser. In this work we study the optimal output of engines subjected to this type of constraints. We find that the details of the engine are irrelevant when the baths are very hot. The efficiency at maximal output is determined only by the nature of the constraint and the temperatures. For some family of constraints the universality features can be expressed using a perturbative approach analogous to the classical analysis, but we also identify constraints cannot be treated with perturbation theory.

Typically in classical engines the equation of state of the working substance is known and the output optimization is done by changing the coupling time to the baths. The output power may change from system to system but it was observed that for some classes of classical engines the efficiency at maximum power has universal features. In particular in [3, 4] it was shown that in the low dissipation limit the efficiency at maximum power satisfies:

$$\frac{\eta_c}{2} \leq \eta_{LD} \leq \frac{\eta_c}{2 - \eta_c}, \quad (1)$$

where η_c is the Carnot efficiency. The same results were obtained in [5, 6] for different thermalization mechanisms. In the low dissipation scenario, the special case where the coupling coefficients to the cold and hot baths is the same (symmetric case) yields the Curzon-Ahlborn [7–9] efficiency,

$$\eta_{CA} = 1 - \sqrt{T_c/T_h}. \quad (2)$$

η_{CA} was originally obtained by applying the Newton heat transfer law. Features of universality appear in the Taylor expansion of the efficiency in terms of the Carnot efficiency. In [10] it was shown that:

$$\eta_{Pmax} = \frac{\eta_c}{2} + \frac{\eta_c^2}{8} + O(\eta_c^3). \quad (3)$$

The $\frac{1}{2}$ factor of the linear term is universal and the second term is universal for systems that have a “left-right” symmetry. For studies of efficiency in different model see [11–14] and references therein.

In this work we study work optimization for quantum Otto engines [15]. The working substance is a single N -level particle that is coupled periodically to hot and cold baths. The properties of this quantum working substance are determined by the level structure of the particle when it is coupled to the hot and to the cold baths. We optimize the level structure to produce maximal work output per cycle. When the cycle time is fixed this is equivalent to power optimization. The classical optimization described earlier can be called “external” as it involves the optimization of the coupling process to the external bath. The maximum power in this case originates from the fact that reaching a thermal equilibrium with the baths is time consuming. Yet our optimization is “internal” as we optimize over the working medium properties (the level structure). We will assume that the baths is coupled for sufficiently long period to effectively reach equilibrium for all practical purposes. This assumption is very reasonable when only one particle needs to be thermalized (and not a whole medium filled with particles). Yet, the analysis here includes the case of partial “swap” thermalization [15] ($\xi \neq 1$). It is remarkable that

for the most basic constraints the results of this internal structure quantum optimization are identical to the classical external coupling optimization.

We consider a generic single particle four-stroke Otto cycle. In the adiabatic strokes the energy levels of the particle (engine) change in time without changing the populations (see discussion in [15] on ways of achieving this in a short time). In the thermal strokes the system is coupled to hot and cold baths. If the system is coupled for periods that exceed a few relaxation times, it is plausible to assume a full thermalization has taken place. As we show in this work, some universal engine-independent features appear in the ultra-hot limit where only the leading order in β (inverse of the temperature) is kept. In some cases, our results hold to order β^2 as well.

The work output of an N -level ultra-hot swap engine is [15]:

$$W_{hot}^{ultra} = \frac{\xi}{2-\xi} \frac{1}{N} [(\beta_c + \beta_h) \mathcal{E}_c \cdot \mathcal{E}_h - \beta_c |\mathcal{E}_c|^2 - \beta_h |\mathcal{E}_h|^2], \quad (4)$$

where $\mathcal{E}_{c(h),i}$ is the i -th cold (hot) energy level of the engine. The energy levels are shifted so that $Mean(\mathcal{E}) = 0$. The work is energy shift invariant but a zero mean lead to a more compact form. The swap parameter $0 \leq \xi \leq 1$ determines the degree of thermalization in the thermal strokes of the engine. When $\xi = 1$ a full thermalization takes place. This case should hold for any interaction that lead to a practically full thermalization regardless of the mechanism that generates it. Before proceeding we note that the norm of the levels in the ultra hot regime is directly related to several key quantities. For example, the internal energy when couple to the one bath is $tr(\rho_b \hat{\mathcal{E}}_b) = \frac{1}{N} \beta_b |\mathcal{E}_b|^2$, the purity is $tr(\rho_b^2) = \frac{1}{N} + \frac{1}{N^2} \beta_b^2 |\mathcal{E}_b|^2$, and the heat capacity is $C_v = \frac{1}{N} \beta_b^2 |\mathcal{E}_b|^2$. Another example for the norm significance will be given later on. In [15] it was shown that once the variance (or norm) of the hot and cold levels are fixed, the maximum work is obtained when the energy vectors are parallel:

$$\mathcal{E}_c = (1 - \chi) \mathcal{E}_h, \quad (5)$$

$$0 \leq \chi \leq \eta_c, \quad (6)$$

where χ , the compression deviation, is related to the compression ratio via $\mathcal{C} = \frac{1}{1-\chi}$. Condition (6) follows from the necessary condition for engine operation in the ultra-hot regime $T_c/T_h \leq |\mathcal{E}_c|/|\mathcal{E}_h| \leq 1$ (see [15]). The exact expression for the efficiency of an Otto engine with uniform compression (5) is [15]:

$$\eta = 1 - |\mathcal{E}_c|/|\mathcal{E}_h| = \chi. \quad (7)$$

Despite the equality of (7) it is useful to separate the notation in order to prevent confusion. The maximal

work in terms of χ and the Carnot efficiency is:

$$W_\chi = \frac{\xi}{2-\xi} \beta_c \chi (\eta_c - \chi) \frac{|\mathcal{E}_h|^2}{N}, \quad (8)$$

where the subscript χ indicates that we have already imposed the necessary but not sufficient optimality condition (5). Notice that $W_\chi(\chi = 0) = 0$ (no compression) and $W_\chi(\chi = \eta_c) = 0$ (reversible limit in Otto engines). Since $|\mathcal{E}_h| \neq 0$, it follows from (8) that a maximum exists in the domain $\chi = \eta \in (0, \eta_c)$. The maximal work in the ultra-hot regime has an inherent universality. It depends only on the norms $|\mathcal{E}_h|^2$ and $|\mathcal{E}_c|^2$ (or $|\mathcal{E}_h|^2$ and the compression ratio). The specific energy levels structure plays no role. All quantum Otto engines [16] with the same energy variance $|\mathcal{E}_h|^2/N, |\mathcal{E}_c|^2/N$ will have the same efficiency and same maximal work per cycle (up to the $\xi/(2-\xi)$ factor in (8)). The finer details of the engine manifest themselves only at colder temperatures.

WORK PER CYCLE OPTIMIZATION

We start with a few important cases that exemplify the kinship to the classical case with very little algebra. First we choose the constraint $|\mathcal{E}_h| = \text{const}$. Applying $\frac{d}{d\chi} W_\chi = 0$ to (8) with fixed $|\mathcal{E}_h|$ yields:

$$\eta_{|\mathcal{E}_h|} = \frac{\eta_c}{2}, \quad (9)$$

which is the lower limit on the efficiency in the low dissipation model (1). On the other hand the opposite constraint $|\mathcal{E}_c| = \text{const}$ ($|\mathcal{E}_h| = \text{const}/(1-\chi)$) yields:

$$\eta_{|\mathcal{E}_c|} = \frac{\eta_c}{2 - \eta_c}, \quad (10)$$

which is the upper limit on the efficiency in the low dissipation model (1). When applying the symmetric constraint $|\mathcal{E}_c| |\mathcal{E}_h| = \text{const}$ then:

$$\eta_{|\mathcal{E}_c| |\mathcal{E}_h|} = \eta_{CA} = 1 - \sqrt{1 - \eta_c}. \quad (11)$$

Although this specific symmetric constraint yields CA efficiency (2), we shall see that symmetry does not necessarily lead to the CA efficiency in quantum Otto engines. The CA efficiency was observed in a specific hot quantum engine in [17]. Another important example follows from the constraint $\alpha |\mathcal{E}_c| + (1-\alpha) |\mathcal{E}_h| = \text{const}$ that yields the maximum power efficiency:

$$\eta_\alpha = \frac{\eta_c}{2 - \alpha \eta_c}. \quad (12)$$

This efficiency form frequently appears in various classical systems such as Brownian engines [12], system operating in the low dissipation limit [4], and system with other thermalization processes [5, 6].

The simple linear constraints studied above can be solved in a closed form. In what follows we explore the low efficiency limit for a general constraint and find universal features.

A GENERAL OPTIMIZATION CONSTRAINT

As an example for a non-trivial physical constraint that is characterized by the energy norms, consider the quantum Otto engine studied in [18, 19]. This engine has four energy levels and it is comprised of two interacting spins and an external time-dependent magnetic field. In order to have the same population in the beginning and at the end of the adiabatic evolution strokes a certain protocol must be applied. Using the optimal protocol in [19], the minimal time for the adiabatic step is proportional to $\frac{1}{|\mathcal{E}_h|} + \frac{1}{|\mathcal{E}_c|}$ (to simplify (24) in [19] we considered the limit $\omega_f, \omega_i \ll j$). Thus, for the engine to operate at the minimal possible time (e.g to maximize the power) the constraint is $\frac{1}{|\mathcal{E}_h|} + \frac{1}{|\mathcal{E}_c|} = \text{const}$. This example shows that time optimization for maximal power by eliminating the quantum non-adiabatic effects, manifest itself as an energy norm constraint. In addition it clarifies that for observing universality there is a justified need for a framework valid for more complicated constraints. Applying $\frac{d}{d\chi} W_\chi = 0$ to (8) we get:

$$\frac{\frac{d}{d\chi} |\mathcal{E}_h|}{|\mathcal{E}_h|} = \frac{(\eta_c - 2\chi)}{2(\chi\eta_c - \chi^2)}. \quad (13)$$

At this point we introduce the constraint function:

$$G(|\mathcal{E}_c|, |\mathcal{E}_h|) = \text{const}. \quad (14)$$

that can describe either an implementation constraint or a design goal. writing:

$$G((1 - \chi) |\mathcal{E}_h(\chi)|, |\mathcal{E}_h(\chi)|) = \text{const}. \quad (15)$$

we get the extra equation needed to find χ . The only limitation on G is that (15) must provide a positive continuous solution for $|\mathcal{E}_h|$ in the domain $0 < \chi < \eta_c$. When $|\mathcal{E}_h(\chi)|$ can be solved explicitly from (15), then it can be used to evaluate the left hand side of (13) and obtain an explicit equation for the optimal χ . Yet, it is simpler to take the derivative of (15), evaluate $\frac{d}{d\chi} |\mathcal{E}_h| / |\mathcal{E}_h|$ and then use it in (13). Even this simpler method is limited to very simple constraints and it is hard to see the underlying universal structure and compare it the classical results. In what follows we explore the low efficiency limit, but before doing so we wish to point out that the solution of (13) and (15) yields an efficiency of the form $\eta = \eta(G, \eta_c)$. That is, an efficiency that depends only on the constraint and on the temperature ratio. It does not depend on the number of levels or on the engine specific details of the energy level structure \mathcal{E}_h . Hence, even without an explicit solution it is clear there is universality to all order in χ for hot quantum Otto engines that are subjected to the some constraint (or requirement).

To the lowest order in χ we can expand:

$$\frac{d}{d\chi} |\mathcal{E}_h| / |\mathcal{E}_h| = A + B\chi. \quad (16)$$

Using (16) in (13) lead to a cubic equation in χ . Since χ is small we use the lowest order solution $\chi = \frac{\eta_c}{2}$ and replace the cubic term by $\chi^3 = \frac{\eta_c^3}{8}$. This yields a quadratic equation that is correct up to order of η_c^3 . The solution is:

$$\eta = \frac{1}{2}\eta_c + a\eta_c^2 + b\eta_c^3 + O(\eta_c^4), \quad (17)$$

$$a = A/4, \quad (18)$$

$$b = B/8. \quad (19)$$

In order to obtain a and b we need to specify a constraint function: To evaluate A and B we expand (15) in powers of χ . Since $G = \sum F_k \chi^k$ is constant in χ , all nonzero order multipliers $F_{i>0}$ should be zero. In particular $F_1 = 0$ yields:

$$\begin{aligned} a &= \frac{1}{4} \left(\frac{d}{d\chi} |\mathcal{E}_h| / |\mathcal{E}_h| \right)_{\chi=0} \\ &= \frac{1}{4} \frac{G_{10}}{G_{10} + G_{01}} \Big|_{\chi=0}, \end{aligned} \quad (20)$$

where the subscript of G specify the order of derivatives with respect to the first and second variable (the values of the variables are omitted for brevity but they are determined by $\chi = 0$: $|\mathcal{E}_c| = |\mathcal{E}_h| = |\mathcal{E}_h|_{\chi=0}$). From (20) two important results immediately follow. First, if the constraint is symmetric $G(|\mathcal{E}_c|, |\mathcal{E}_h|) = G(|\mathcal{E}_h|, |\mathcal{E}_c|)$, then $G_{10} = G_{01}$ for $\chi = 0$ and therefore:

$$a_{sym} = \frac{1}{8}. \quad (21)$$

The second result that follows from (20) concerns the asymmetric case where $G_{10} \neq G_{01}$. If G_{10} and G_{01} have the same sign then:

$$0 \leq a_{sign} \leq \frac{1}{4}. \quad (22)$$

The two extreme values 0 and $\frac{1}{4}$ appear in the $|\mathcal{E}_h| = \text{const}$ and $|\mathcal{E}_c| = \text{const}$ studied earlier.

Notice that in contrast to the classical power optimization studied in [3], in the quantum work optimization studied here the functions $\eta_{|\mathcal{E}_c|}$ is not necessarily an upper bound on the efficiency. For example, this is true if the sign of G_{10} is different from that of G_{01} . This can be seen by comparing the leading order of the two cases:

$$\eta_{quantum} = \frac{\eta_c}{2} + \frac{\eta_c^2}{4(1 + \frac{G_{01}}{G_{10}})} + O(\eta_c^3) \quad (23)$$

$$\eta_{LD} = \frac{\eta_c}{2} + \frac{\eta_c^2}{4(1 + \frac{\sqrt{\Sigma_c}}{\sqrt{\Sigma_h}})} + O(\eta_c^3) \quad (24)$$

where $\Sigma_{c,h}$ are the baths relaxation time scales [3]. Since $\Sigma_c \geq 0, \Sigma_h \geq 0$ it follows that $a \leq 1/4$ (for $|\mathcal{E}_c| = \text{const}$ $a = 1/4$). In contrast in the quantum case a can be larger if G_{01}/G_{10} is smaller than zero. For example, consider the constraint $|\mathcal{E}_c| - (1-d)|\mathcal{E}_h| = \text{const}$. $G_{01} = d - 1$, $G_{10} = 1$ so quadratic term is $\frac{1}{4d}\eta_c^2$. For $d = 1$ we get the expected $\frac{1}{4}$ for $|\mathcal{E}_c| = \text{const}$, but for smaller d , $a > 1/4$. Note that d should satisfy $d > \eta_c$. When $d = \eta_c$ the Taylor series no longer converges. Physically, beyond this point the solution is no longer an engine. A more dramatic non-classical behavior appears when imposing the constraint $\frac{s}{\eta_c}|\mathcal{E}_c| + (1 - \frac{s}{\eta_c})|\mathcal{E}_h| = \text{const}$. This is just the α constraint solved before (12) with $\alpha = \frac{s}{\eta_c}$. This constraint leads to a positive definite $|\mathcal{E}_h|$ for any $-\infty < s < 1$. This condition also ensures that the device operates as an engine ($W > 0$). Using (12) we get:

$$\eta_s = \frac{\eta_c}{2-s}. \quad (25)$$

This is different from the factor of half predicted for the linear term from classical linear response theory. In particular, the efficiency is not bounded by the range obtained from the low dissipation theory (1) [3]. For $s = 1$ the efficiency is equal to Carnot but $|\mathcal{E}_h| = 0$ so as expected the work is zero. Notice that this constraint is not of the form (14) as it involves the temperatures as well. Consequently, formulas (20) and (23) (as well as (27) that follows) are not valid. This can be understood by writing (12) as a series using $\frac{1}{1-q} = \sum_{j=0}^{\infty} q^j$. When $s = \frac{q}{\eta_c}$ all powers collapse into a linear power of η_c . Therefore, the truncated perturbation analysis carried out before can never give the right result for this type of order changing constraints.

NEXT ORDER FOR SYMMETRIC CONSTRAINTS

we use the $F_2 = 0$ condition from $\text{const} = G = F_0 + F_1\chi + \frac{1}{2}F_2\chi^2 + O(\chi^3)$ and get for the symmetric case ($G_{ij} = G_{ji}$):

$$\frac{\frac{d}{d\chi}|\mathcal{E}_h|}{|\mathcal{E}_h|} = \frac{1}{2} + \frac{1}{4}\left[1 + \frac{|\mathcal{E}_h|(G_{11} - G_{20})}{G_{10}}\right]_{\chi=0}\chi \quad (26)$$

The multiplier of the linear term is B and therefore:

$$\begin{aligned} \eta_{sym} &= \frac{1}{2}\eta_c + \frac{1}{8}\eta_c^2 \\ &+ \frac{1}{32}\left[1 + \frac{|\mathcal{E}_h|(G_{11} - G_{20})}{G_{10}}\right]_{\chi=0}\eta_c^3 + O(\eta_c^4) \end{aligned} \quad (27)$$

For example for the CA constraint $|\mathcal{E}_c||\mathcal{E}_h| = \text{const}$, $G_{11} = 1$, $G_{20} = 0$, $G_{10} = |\mathcal{E}_h|$ and indeed we get the correct factor $\frac{1}{16}\eta_c^3$. As a second example consider

the efficiency $\eta_{\alpha=1/2}$ (12) obtained from the constraint $|\mathcal{E}_c| + |\mathcal{E}_h| = \text{const}$. In this case $G_{11} = G_{20} = 0$ so the multiplier of the cubic term is $1/32$ as can be verified from the exact expression for the efficiency. Using the same methods a similar (yet considerably more cumbersome) formula can be written for the non-symmetric case.

EXTENSION TO COLDER ENGINES

Surprisingly the next order in β only adds the following leading order terms to the work:

$$\begin{aligned} \frac{\xi}{2-\xi} \frac{1}{N} \sum_{i=1}^N &\left[\frac{1}{2}\beta_c^2 \mathcal{E}_{c,i}^3 + \frac{1}{2}\beta_h^2 \mathcal{E}_{h,i}^3 \right. \\ &\left. - \frac{1}{2}\beta_c^2 \mathcal{E}_{c,i}^2 \mathcal{E}_{h,i} - \frac{1}{2}\beta_h^2 \mathcal{E}_{h,i}^2 \mathcal{E}_{c,i} \right] \end{aligned} \quad (28)$$

In principle, it complicates the optimization, however if the $\mathcal{E}_c, \mathcal{E}_h$ are symmetric with respect to zero then each term individually sums up to zero and all the results previously obtained still hold. In particular (28) is always zero for a two-level systems and systems with evenly-space spectrum.

We have studied internal optimization of hot quantum Otto engines. Universal features of the efficiency were identified. For some optimization constraints the efficiencies at maximal work are the same as the efficiency at maximum power in the low dissipation limit. Yet, we find constraints for which the efficiencies deviate from the classical results, as they cannot be obtained from perturbative analysis. In the present case the optimization is with respect to the internal properties of the working fluid, while in the low dissipation limit the power is optimized with respect to the heat transport. It is interesting to see if similar universality appears in different engines (e.g. continuous engines) and in different operating regimes.

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